Spin-Transfer Torque on a Single Magnetic Adatom

F. Delgado, J. J. Palacios, and J. Fernández-Rossier

Departamento de Física Aplicada, Universidad de Alicante, San Vicente del Raspeig, 03690, Spain
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We theoretically show how the spin orientation of a single magnetic adatom can be controlled by spin polarized electrons in a scanning tunneling microscope configuration. The underlying physical mechanism is spin assisted inelastic tunneling. By changing the direction of the applied current, the orientation of the magnetic adatom can be completely reversed on a time scale that ranges from a few nanoseconds to microseconds, depending on bias and temperature. The changes in the adatom magnetization direction are, in turn, reflected in the tunneling conductance.

There is now a fast growing interest in controlling the spin orientation of a single or few magnetic atoms in a solid state environment for future spintronics and quantum information devices. So far this has only been achieved using optical methods [1]. When a current flows through a magnetic region it becomes spin polarized due to exchange coupling between transport electrons and localized magnetic moments. The backaction of transport electrons on the magnetic moment, known as spin-transfer torque [2], can be used to rotate the magnetization in nanopillars made of 10^6 atoms [3]. The magnetization of such a large number of atoms can be described with a single classical vector, and the current driven magnetization switching is properly modeled by Landau-Lifshtitz equations extended with the spin-transfer term proposed by Slonczewski [2]. Current induced magnetization switching has been reported in much smaller nanomagnets, made of 100 atoms [4], but still in the semiclassical domain.

In this Letter we theoretically show how a spin polarized current can be used to manipulate the spin state of a single transition metal atom deposited on an insulating monolayer on top of a metallic surface [see Fig. 1(a)]. The proposed implementation combines two alternative strategies used so far to probe the spin of a single atom on a surface: inelastic electron tunnel spectroscopy (IETS) with non-magnetic tips on one side and a spin polarized tunneling current on the other. The first technique has demonstrated that conveniently isolated Mn, Fe, and Co adatoms have quantized spin angular momentum along a well-defined magnetic easy axis [5–8]. These experiments also demonstrate that transport electrons and local spin are exchange coupled [9–11]. In contrast, experiments with ferromagnetic tips are based upon the sensitivity of conductance to the relative spin orientation of the tip and adatom (magnetoresistance) [12].

Here we present a fully quantum mechanical theoretical analysis showing that, under the influence of spin polarized tunneling current, the spin of a single magnetic atom can be directed either parallel or antiparallel to the magnetic moment of the tip (or the surface). When the current is spin polarized along a given direction $\vec{n}$, because either the tip

or the substrate is ferromagnetic, a fraction of the tunneling electrons exchange one unit of spin with the magnetic adatom. This induces a net transfer of spin along $\vec{n}$ towards the magnetic atom. This current driven spin torque competes with the adatom spin relaxation provided by its weak coupling to the tip and substrate. The sign of the transfer is determined by the direction of the current whereas the efficiency is determined by the magnitude of the current.

In order to study the spin dynamics of the magnetic adatom under the influence of the spin polarized tunneling electrons we derive and solve the master equation for the eigenstates $|M\rangle$ of the single ion spin Hamiltonian

$$\mathcal{H}_S = DS_z'^2 + E(S_x'^2 - S_y'^2). \tag{1}$$

Thus, the local spin is described quantum mechanically, in contrast to previous works [13,14]. This is crucial to account for the IETS experiments [5]. Here the prime
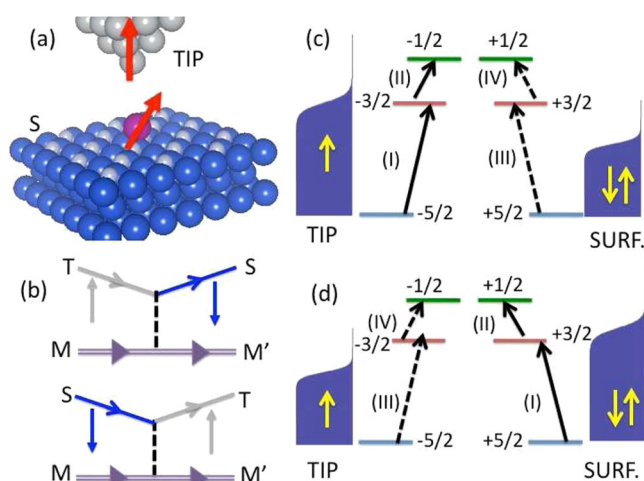

FIG. 1 (color online). (a) Scheme of the proposed setup: a magnetic STM tip and a magnetic adatom on an insulating monolayer deposited on a metal. (b) Two of the spin assisted tunneling events of Eq. (2). Spin transitions when electrons flow from tip to surface (c) and from surface to tip (d). Dashed transitions (III) and (IV) are less efficient when the tip is polarized (see text).

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denotes that the spin quantization axis is chosen with z perpendicular to the surface. For convenience, we choose the quantization axis of all the spins in the Hamiltonian along direction $\vec{n}$ which makes it necessary to rotate $\mathcal{H}_S$ when $\vec{n}$ is not perpendicular to the surface. The value of the total spin S^2 and the magnetic anisotropy coefficients D and E change from atom to atom and also depend on the substrate [5,6].

The scattering rates between states with different spin projection $|M\rangle$ arise from the exchange interaction of the adatom spin to delocalized electrons in tip and surface, hereafter denoted as the reservoirs and labeled with the indices $\eta = T, S$. The total Hamiltonian of the adatom coupled to the reservoirs reads $\mathcal{H} = \mathcal{H}_{\text{tip}} + \mathcal{H}_{\text{sur}} + \mathcal{H}_S + \mathcal{V}$. The first three terms describe the tip, surface, and adatom as decoupled systems, whereas the $\mathcal{V}$ term introduces interactions between them. The first term describes the electrons in the ferromagnetic tip magnetized along the direction $\vec{n}$. The second term is the Hamiltonian of the nonmagnetic electrons of the metallic surface. Thus, the quantum numbers of the transport electrons are their momentum k, spin along the $\vec{n}$ axis, σ, and reservoir $\eta = $ tip, sur. With this notation we write $\mathcal{H}_{\text{tip}} + \mathcal{H}_{\text{sur}} = \sum_{k,\sigma,\eta} \epsilon_{\sigma\eta}(k) c_{k\sigma\eta}^\dagger c_{k\sigma\eta}$. Since we consider a nonmagnetic surface, we have $\epsilon_{\sigma,S}(k) = \epsilon_S(k)$. All the results of this Letter are trivially generalized to the case of a nonmagnetic tip and a magnetic surface.

The coupling of the atomic spin $\vec{S}$ and the conducting reservoirs has the form [15]

$$\mathcal{V} = \sum_{\alpha,k,k',\sigma,\sigma',\eta,\eta'} T_{\eta,\eta',\alpha}(k,k') \frac{\tau_{\sigma\sigma'}^{(\alpha)}}{2} \hat{S}_\alpha c_{k\sigma\eta}^\dagger c_{k'\sigma'\eta'}, \quad (2)$$

where the index α runs over 4 values, $a = x, y, z$, and $\alpha = 0$. We use $\tau^{(a)}$ and $\hat{S}_a$ for the Pauli matrices and the spin operators in the $\vec{n}$ frame, while $\hat{S}_0 = I$ is the identity matrix. $T_{\eta,\eta',\alpha}(k,k')$ for $\alpha = x, y, z$ is the exchange-tunneling interaction between the localized spin and the transport electrons and potential scattering for $\alpha = 0$. Attending to the nature of the initial and final electrode, Eq. (2) describes four types of exchange interaction, two of which contribute to the current, the other two conserving the charge difference between tip and surface. The former are crucial to account for the magnetic IETS [9] and tend to "heat" the spin of the adatom. The other two provide an efficient cooling mechanism, through a Korringa-like spin relaxation, and were not included in previous work [9–11]. Following Anderson [16], we assume that (2) arises from kinetic exchange. The momentum dependence of $T_{\eta,\eta',\alpha}(k,k')$ can have important consequences in the conductance profile [17] in an energy scale of eV, so it can be safely neglected in IETS. We thus parametrize $T_{\eta,\eta',\alpha=0}(k,k') = v_\eta v_{\eta'} T_0$ and $T_{\eta,\eta',a}(k,k') = v_\eta v_{\eta'} T_S$, where T_S is the same for $a = x, y, z$ and v_{sur} and v_{tip} are dimensionless factors that scale as the surface-adatom and

tip-adatom hopping integrals. This parametrization sets a relation between spin torque and spin relaxation.

The occupation of the spin states $|M\rangle$, P_M are governed by the master equation

$$\frac{dP_M}{dt} = \sum_{M',\eta\eta'} P_{M'} W_{M',M}^{\eta'\to\eta} - P_M \sum_{M',\eta\eta'} W_{M,M'}^{\eta\to\eta'}, \quad (3)$$

where $W_{M,M'}^{\eta\to\eta'}$ are the scattering rates from state M to M' induced by interaction with a quasiparticle which is initially in reservoir η and ends up in η'. Equation (3) does not include spin coherences. This approximation is good provided that spin decoherence is faster than spin relaxation, which is known to be the case due to hyperfine coupling [1] in Mn atom. After some algebra, the scattering rates can be written as

$$W_{M,M'}^{\eta\to\eta'} = \frac{\pi |T_S v_\eta v_{\eta'}|^2}{\hbar} \mathcal{G}(\Delta_{M,M} + \mu_\eta - \mu_{\eta'}) \Sigma_{M,M'}^{\eta\eta'}, \quad (4)$$

where $\mathcal{G}(\omega) \equiv \omega(1 - e^{-\beta\omega})^{-1}$ are the phase space factors associated to quasiparticle scattering, $\Delta_{M,M'} = E_M - E_{M'}$ is the energy change of the atom, μ_η is the chemical potential of electrode η, and $\Sigma_{M,M'}^{\eta,\eta'}$ are spin matrix elements

$$2\Sigma_{M,M'}^{\eta\eta'} = |\mathcal{S}_z^{M,M'}|^2 (\rho_{\eta\uparrow}\rho_{\eta'\uparrow} + \rho_{\eta\downarrow}\rho_{\eta'\downarrow}) + |\mathcal{S}_+^{M,M'}|^2 \rho_{\eta\downarrow}\rho_{\eta'\uparrow} + |\mathcal{S}_-^{M,M'}|^2 \rho_{\eta\uparrow}\rho_{\eta'\downarrow}, \quad (5)$$

where $\mathcal{S}_a^{M,M'} = \langle M|S_a|M'\rangle$ and $\rho_{\eta,\sigma}$ is the density of states at the Fermi energy for spin σ in the electrode η. These equations show that, for a ferromagnetic tip, spin flip and spin conserving rates are different, in contrast to the case of a nonmagnetic tip [9]. The rates that induce changes in the adatom spin population are all proportional to T_S^2 and can be classified in three groups: intratip, intrasurface, and tip-surface rates ($\propto v_{\text{tip}}^4$, $\propto v_{\text{sur}}^4$, and $\propto v_{\text{tip}}^2 v_{\text{sur}}^2$, respectively). In the first two, the capability to transfer energy to the magnetic atom is given by the temperature, being the release of energy from the atom to the electrodes always allowed. In contrast, the rates carrying current can transfer energy to the atom even at zero temperature, provided that there is a bias voltage $eV = \mu_S - \mu_T$.

On top of the T_S^2 rates, there are scattering processes of order T_0^2 and $T_0 T_S$ that do not change the occupations but contribute to the current. Evaluated to the same second order in $\mathcal{V}$ as the rates in the master equation, the expression of the current has three terms, $I = I_0 + I_{MR} + I_{IN}$. The first term is elastic and spin independent. The second is the elastic but sensitive to the relative spin orientation of the adatom and the tip magnetic moment. The third term comes from the inelastic exchange processes being proportional to T_S^2. The expressions for the three contributions to the current, analogous to those derived elsewhere [10], are

$$I_0 + I_{MR} = -\frac{2}{e} G_0 [1 + x\langle S_z\rangle \mathcal{P}_T i_-(-eV)] \quad (6)$$

$$I_{IN} = -\frac{G_S}{e} \sum_{M,M'} [i_-(\Delta_{M,M'} - eV) \sum_a |\mathcal{S}_a^{M,M'}|^2$$

$$+ \mathcal{P}_T i_+(\Delta_{M,M'} - eV) \, \text{Im}(\mathcal{S}_x^{M,M'} \mathcal{S}_y^{M',M})] P_M(V).$$

$$(7)$$

Here $G_0 \equiv \frac{e^2 \pi \rho_T \rho_S}{4\hbar} |T_0 v_{\text{tip}} v_{\text{sur}}|^2$ is the elastic conductance of the junction while $G_S = x^2 G_0$, with $x = T_S/T_0$ the relative intensity of the inelastic channel. We define the spin polarization of the tip $\mathcal{P}_T = (\rho_{T\uparrow} - \rho_{T\downarrow})/(\rho_{T\uparrow} + \rho_{T\downarrow})$. Functions $i_\pm$ are defined as $i_\pm(\Delta_{M,M'} - eV) = \mathcal{G}(\Delta_{M,M'} - eV) \pm \mathcal{G}(\Delta_{M,M'} + eV)$. The average adatom magnetization along the tip magnetization axis is $\langle S_z \rangle = \sum_M P_M(V) \langle M|S_z|M \rangle$ and depends on the bias voltage, the central result of this Letter. Importantly, the magnetoresistive contribution to the elastic current permits one to track changes in magnetization. Although x varies from system to system, we take $x = 1$ close to experimental values [5].

The inelastic contribution also has two terms. The first inelastic term, independent of $\mathcal{P}_T$, is proportional to i_-, whose derivative with respect to V gives the characteristic inelastic conductance steps as $|eV|$ goes across $|\Delta_{M,M'}|$. By contrast, the $\mathcal{P}_T$ dependent term, proportional to i_+, yields steps at the excitation energies of opposite sign as the polarity of the bias is reversed. Both the elastic and inelastic term proportional to $\mathcal{P}_T$ can produce a dI/dV which is not an even function of bias.

We can now address the main question of this Letter: How does a spin polarized tunneling current affect the magnetization of a single adatom? We consider first the simplest situation, where the magnetic moment of the tip is parallel to the easy axis of the single atom. We choose a single Mn atom on a Cu_2N surface, which in the case of nonmagnetic tip is very well characterized experimentally [5] and theoretically [9–11,18]. The spin of the Mn atom in this situation is $S = 5/2$ with $D = -0.039$ meV and $E = 0.007$ meV. Since $E \ll |D|$ we can limit our qualitative discussion to the case $E = 0$, so that the eigenstates of $\mathcal{H}_S$ are also eigenstates of S_z. The numerical simulations are done with $E \neq 0$ and do not change qualitatively. In the absence of applied magnetic field and at temperatures $k_b T \ll 4|D|$, the equilibrium distribution is such that the two ground states, $S_z = \pm 5/2$, are equally likely and $\langle S_s \rangle^{Eq} = 0$.

The nonequilibrium dynamics of the atom depends on a number of parameters that can be tuned experimentally, such as the bias voltage, the temperature, and the ratio $r \equiv \frac{v_{\text{tip}}}{v_{\text{sur}}}$. The latter depends on the tip-adatom distance. As a general rule, the processes that drive the magnetic adatom out of equilibrium are proportional to $v_{\text{tip}}^2 v_{\text{sur}}^2$ whereas the processes that cool the spin down (provided that $k_b T < e|V|$) are proportional to $v_{\text{tip}}^4 + v_{\text{sur}}^4$. Thus, the non-equilibrium effects are higher as r increases. We always take $r < 1$.

In Fig. 2(a) we plot the *steady state* average magnetization of the Mn atom for $\mathcal{P}_T = -1$ and $v_s = 2v_T = 1$ and
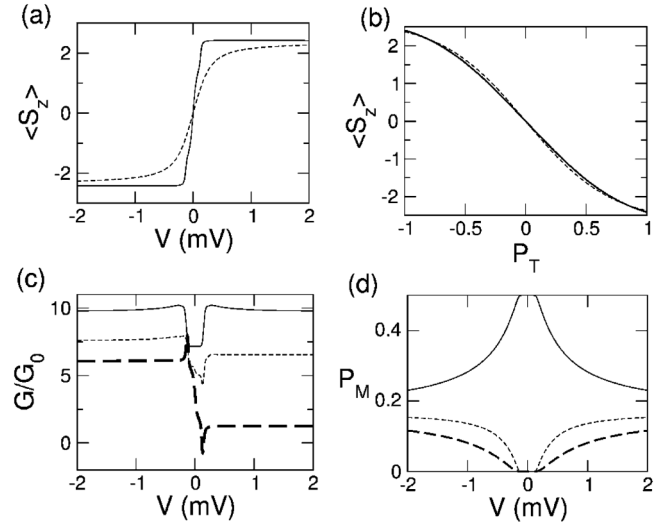

FIG. 2. (a) Average magnetization $\langle S_z \rangle$ versus applied bias for $T = 1$ K (dashed line) and $T = 0.1$ K (solid line). (b) Average magnetization after saturation ($eV = 5$ meV) versus tip polarization for the same two temperatures. (c) dI/dV for single Mn in Cu_2N surface probed with a nonpolarized tip (solid line) and two different tip polarizations, $\mathcal{P}_T = -1/3$ (thin dashed line) and $\mathcal{P}_T = -1$ (thick dashed line) for a fixed temperature $T = 0.1$ K. (d) Variation of the populations P_M with applied bias for nonpolarized tip and $T = 0.1$ K.

two temperatures, $T = 1$ K and $T = 0.1$ K, as obtained from solving Eq. (3). The tip polarization was assumed parallel to the Mn easy axis. The result has three outstanding features. First, the magnetization of the atom can be reversed from parallel to antiparallel just by electrical means [Fig. 2(a)]. Second, the saturation magnetization can take very large values, which increase up to 100% for $E = 0$ as the degree of spin polarization of the tip increases [see Fig. 2(b)]. Third, the magnetization switch produces a large asymmetry between positive and negative bias conductance $G = dI/dV$ [Fig. 2(c)] which would be the experimental evidence of the spin transfer.

The magnetization shown in Figs. 2(a) and 2(b) arises from the competition between spin transfer from the spin polarized current to the atom and spin relaxation. The microscopic spin-transfer events, depicted in Figs. 1(b)–1(d), are the same than those resulting in steps in IETS [5,9]. In the case of Mn atom probed by nonmagnetic tip, a single step has been reported [5], related to the spin increasing transitions $-5/2 \rightarrow -3/2$ and its time reversal counterpart, the spin decreasing transition $+5/2 \rightarrow +3/2$, both with energy $4|D|$ [see Figs. 1(c) and 1(d)]. For non-magnetic electrodes there is no net spin transfer because the rates (4) of these two processes are identical. In contrast, net spin transfer occurs when the tip is magnetic and these two processes have different rates. This is more easily seen in an extreme case $\mathcal{P}_T = 1$, a half-metallic tip ($\rho_{T\downarrow} = 0$). Then, spin flip assisted tunneling from tip to surface can only decrease the transport spin [upper diagram in Fig. 1(b)], *increasing* the spin of the magnetic
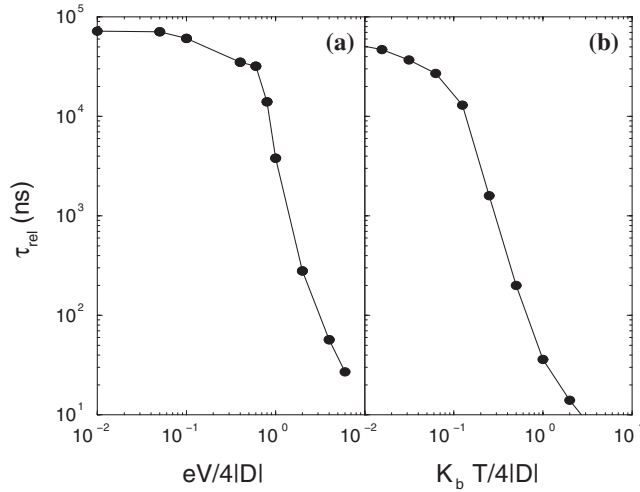
FIG. 3. Switching time $\tau_{\rm rel}$ for $\mathcal{P}_T = -1$, $\nu_S = 1$, and $\nu_T = 0.5$. (a) $\tau_{\rm rel}$ as a function of applied bias V for $T = 0.1$ K and (b) as a function of temperature for $eV = 2|D|$.

adatom [processes (I) and (II) in Fig. 1(c)] whereas processes (III) and (IV) [Fig. 1(c)] are not allowed, or for nonfully polarized tips, partly suppressed. When the bias is reversed, electrons flow from the surface to the tip. In this case, $\rho_{T\downarrow} = 0$ implies that surface-tip spin-flip assisted tunneling can only increase the transport spin [lower diagram in Fig. 1(b)], *decreasing* the adatom spin [processes (I) and (II) in Fig. 1(d)].

In the case of nonmagnetic tip, our theory predicts a nonequilibrium effect which has been already observed experimentally [6]: the small decay of dI/dV for eV larger than the inelastic threshold. The spin-flip assisted events [Figs. 1(b)–1(d)] deplete the ground state doublet in favor of the first excited state doublet [Fig. 2(d)]. This opens two new transport channels ($\pm 3/2 \rightarrow \pm 1/2$) [processes (II) and (IV) in Figs. 1(c) and 1(d)] which, in this case, happens to be less efficient than the channels $\pm 5/2 \rightarrow \pm 3/2$ [processes (I) and (III) in Figs. 1(c) and 1(d)]. As the bias increases above $4|D|$, the efficient inelastic transitions [(I), (III)] are replaced by the less efficient transitions [(II), (IV)], decreasing the inelastic contribution to dI/dV.

The spin-transfer events that "heat" the adatom require that a quasiparticle has an excess energy larger than $4|D|$. They compete with spin cooling events (order $\nu_{\rm tip}^4$, $\nu_{\rm sur}^4$) that are always available. At $T = 0$, the current induces changes in the magnetization only for bias larger than the inelastic threshold $4|D|$. At finite temperature there are always quasiparticles thermally activated above the $4|D|$ threshold and they are enough to induce the magnetization in the atom, even for $eV < 4|D|$, provided that a sufficiently long time is used in the process. In Fig. 3 we show how the time scale necessary for the switching depends dramatically both on eV and k_bT: the switching time can decrease by up to 4 orders of magnitude as either the bias

goes above $4|D|$ or the temperature is raised above $4|D|/k_b$.

Finally, we have studied the effect of the deviations of the magnetization axis $\vec{n}$ with respect to the adatom easy axis. Curves similar to Fig. 2(a) are obtained for the average magnetization of the adatom along $\vec{n}$ as a function of eV, but the saturation magnetization at high bias is a decreasing function of the angle formed by $\vec{n}$ and the adatom easy axis. The efficiency of the spin transfer is minimal when $\vec{n}$ is perpendicular to the adatom easy axis but still can reach 0.6.

In conclusion we have shown that the spin of a single magnetic adatom can be polarized, reversed, and monitored by means of spin polarized currents in the STM configuration. The time scale for the single spin switching can be as quick as a few nanoseconds. Our proposal adds the possibility of single spin control to the wide range of uses of STM in the field of nanospintronics [5,6]. This possibility is based on nonequilibrium processes and differs from recent work in which switching is achieved by a change of sign of the equilibrium tip-adatom exchange interaction [19].

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